COMPARATIVE PROPERTIES OF SOME TIME DIFFERENCING SCHEMES FOR LINEAR AND NONLINEAR OSCILLATIONS

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ABSTRACT

The properties of 13 computational methods for the integration of first-order differential equations in time are studied. Special attention is given to the representation of periodic fluctuations in a simple spectral baroclinic model of the atmosphere. Errors in the energy, three dimensional scale, and frequency for linear and nonlinear oscillations are evaluated.

Comparisons of both one-step and two-step methods are made. It is found that the two-step schemes compare favorably with one-step methods only when given the advantage of a smaller time increment. Even then, it is concluded that certain one-step procedures incorporating two or more extrapolations over each constant increment of time produce errors which grow most slowly. With small time increments, these errors are generally made smallest by increasing the number of time extrapolations at each step rather than by decreasing the time increment.

1. INTRODUCTION

The continued development of numerical modeling in recent years has produced insight into the mechanisms of various atmospheric phenomena. The broadened spectrum of physical problems has been accompanied by widened investigations into appropriate numerical methods. Impressive advances in the area of space differencing have resulted [1]. On the other hand, meteorological interest in time-differencing procedures has usually been limited to spectral studies of geophysical circulation models (Bryan [3]; Lorenz [13]; Veronis [17]). However, Lilly [10] has suggested that time-differencing methods will now assume a new significance as a consequence of the advances in space-differencing methods. Developments in this area would appear to be especially important for studies of the large-scale climate and its long-period fluctuations.

The purpose of this paper is to present comparative properties of a number of time-differencing schemes designed to handle atmospheric-like oscillations. To a large extent, the methods considered here supplement those discussed by Kurihara [9] and Lilly [10]. In this paper, major attention is given to "one-step" or "deterministic" schemes whereby the solution at a given time step depends only upon the single state of the system at the preceding time step. Such methods are unlike "multistep" methods which often produce nonphysical "parasitic" solutions. However, the suppression of truncation errors in one step methods cannot be accomplished by the use of past solution information, as in the case of multistep methods. Thus, the deterministic scheme must develop greater accuracy by generating approximate states (usually in the future, through the use of at least one forward difference). As will be seen later, the extra work often appears to be worth the extra effort for the one step methods.

In section 2, the exact linear and nonlinear characteristics of a maximally simplified baroclinic model described by three spectral variables are presented. The comparative performances of 10 different one step computational schemes in this model are given in section 3. Section 4 demonstrates that reduction of the time increment Δt is not always the best way to increase accuracy for one step schemes. Section 5 summarizes the properties of three different two step methods. Concluding remarks are contained in section 6.

2. SPECTRAL MODEL OSCILLATIONS

The governing laws for numerical models may often be expressed as a system of first-order ordinary differential equations in time t:

$$\frac{dx_i(t)}{dt}=f_i(x_1, x_2, \ldots, x_M; t). \tag{2.1}$$

Here, $i=1, 2, \ldots, M$. The elements x_i denote the dependent variables at specific points in grid point or wave number space. Included in the functions f_i are quadratic representations of the energy-conserving advective processes.

With given initial conditions, the finite difference approximation to the system (2.1) yields a solution which eventually departs from the exact solution. A measure of the truncation error is given by the order of the last term in which the Taylor Series expansion of (2.1) and its finite difference form agree. This order of accuracy characterizes the local generation of error but is not helpful in describing the accumulation of error over a length of time. Instead, we study the computational

[1] Portions of this study were taken from a Ph. D. thesis submitted to the Dept. of Meteorology, Massachusetts Institute of Technology.

stability of solutions for a particular numerical model. The stability properties are indicative of integrated errors and hence depend upon the character of the solution itself.

We confine ourselves to studying simple linear and nonlinear systems that exhibit periodic fluctuations. A similar approach has been followed by Lilly [10]. A particularly simple system arises from the spectral form of a two-level quasi-geostrophic model with fixed stability. In the case of adiabatic, frictionless flow, the equations have been given by Lorenz [12]. With slight changes in scaling and definitions, these contain the following energetically complete subset:

$$\frac{d\theta_Z}{dt}=-C(1+B_Z)^{-1}\theta_W\psi_W$$

$$\frac{d\theta_W}{dt}=+C(1+B_W)^{-1}(1+B_Z-B_W)\theta_Z\psi_W$$

$$\frac{d\psi_W}{dt}=-CB_W^{-1}(B_Z-B_W)\theta_Z\theta_W. \tag{2.2}$$

Here, ψ and θ are nondimensional representations of the vertically averaged ("barotropic") and vertical shear ("baroclinic") flows, respectively. t is nondimensional time. The static stability $\bar{\sigma}$ is contained in the parameters $B_Z=\bar{\sigma}a_Z^2$ and $B_W=\bar{\sigma}a_W^2$, where $a_Z^2=1.000$ and $a_W^2=1.444444$ are effectively squared wave numbers. The subscripts Z and W refer to the zonal and wave modes, respectively. $C=+0.8002814$ is the interaction coefficient for this set.

With $\bar{\sigma}=0.10$ and initial conditions $\theta_Z(0)=+0.1000$, $\theta_W(0)=+0.0349$, and $\psi_W(0)=0.0000$, an exact solution to the set (2.2) is given in terms of elliptic functions of time (Lorenz [11]). The solution is

$$\theta_Z(t)=+0.1000\ \mathrm{sn}\ (ht+K)$$
$$\theta_W(t)=+0.1020\ \mathrm{dn}\ (ht+K)$$
$$\psi_W(t)=-0.0582\ \mathrm{cn}\ (ht+K) \tag{2.3}$$

where $K=2.5046$ and $h=+0.0406$. This solution exhibits growth of the initially small wave disturbance variables θ_W and ψ_W at the expense of θ_Z; θ_Z decreases to zero and then becomes negative. The vertical tilt of the fully developed wave then changes sign, producing a meridional heat flux which brings the system back to its original state after a nondimensional length of time $4K/h=247.2$.

While this period is the fundamental one for the system, Fourier analysis of the elliptic solutions shows that the nonlinearities produce higher frequencies in abundance (Davis [4]). These high frequencies are associated with transitional time scales much shorter than the fundamental period of oscillation, and arise from the initial wave growth and its subsequent feedback onto the zonal flow. Such sudden changes occurring in the midst of otherwise slow variations provide a stringent test of any computational scheme.

These solutions specify unique amplitudes for each fluctuating variable at all times. For the later computational tests it is convenient to define certain quadratic quantities which do not change in time in the case of the exact solution. The first of these is the sum of the available potential energy and the kinetic energy:

$$E=\frac{1}{2\bar{\sigma}}[\theta_Z^2+\theta_W^2]+\frac{1}{2}[a_Z^2\theta_Z^2+a_W^2(\theta_W^2+\psi_W^2)]. \tag{2.4}$$

The total squared potential vorticity

$$V=[\theta_Z(a_Z^2+\bar{\sigma}^{-1})]^2+[\theta_W(a_W^2+\bar{\sigma}^{-1})]^2+[\psi_W a_W^2]^2, \tag{2.5}$$

also a constant, is used with E to define the second quantity $S=V/E$. S is also invariant; it has the "units" of a_Z^2, a_W^2, or $\bar{\sigma}^{-1}$ and thus is a measure of the three dimensional scale of the flow.[2] We see that E and S are physically meaningful parameters which measure the gross amplitude of the system and the spectral distribution of amplitudes, respectively.

It is important to realize that the period of the nonlinear oscillation is not independent of these quantities; with these quadratic interactions, increases in amplitude result in proportionately higher frequencies.[3] To see this, suppose the amplitude of each variable is initially altered by the same multiplicative factor β. Then E and V are altered by β^2, while S remains unchanged. It is evident in the paper by Lorenz [11] that h^2 is proportional to a linear combination of E and V; hence h is increased by the factor β. K is uninfluenced by β. Thus the period $4K/h$ varies as β^{-1}.

The above features are useful tests of computational schemes for a nonlinear system. However, the analysis of a linear system is also helpful, and is more simply accomplished. In the limit $\bar{\sigma}\to\infty$, baroclinic instability of θ_Z is suppressed and the set (2.2) reduces to

$$\frac{d\theta_Z}{dt}=0$$

$$\frac{d\theta_W}{dt}=-C\left(\frac{a_W^2-a_Z^2}{a_W^2}\right)\theta_Z\psi_W$$

$$\frac{d\psi_W}{dt}=+C\left(\frac{a_W^2-a_Z^2}{a_W^2}\right)\theta_Z\theta_W. \tag{2.6}$$

Equation (2.6) is of the linear form

$$\frac{d\chi}{dt}=i\omega\chi \tag{2.7}$$

where $\chi=\theta_W+i\psi_W$, $i=\sqrt{(-1)}$, and $\omega^2=C^2\left(\frac{a_W^2-a_Z^2}{a_W^2}\right)^2\theta_W^2$.

The solution to (2.7) with initial conditions $\chi(0)=\eta$ can be written as $\chi^{(n)}=G^n\eta$ (2.8), where $\chi^{(n)}$ stands for χ evaluated at times $t=t_0+n\Delta t$. G here has the properties $|G|=1$ and $\arg(G)=p$. We note that p alone determines the frequency of this linear oscillation; the frequency is thus independent of amplitude $|\eta|$, in contrast to the nonlinear case. $p=(\omega\Delta t)$ is generally small; it measures the constant increment Δt against the period of oscillation $2\pi/\omega$.

[2] In barotropic flows such as those considered by Lorenz [11], Lilly [10], and F]ørtoft [5], the "vertical scale" is fixed and S then describes the two-dimensional scale associated with the horizontal flow structure.

[3] This interrelation appears to provide a mechanism for the rapid growth of errors in the later stages, for by shortening the oscillation period the amplitude error can grow all the faster having once reached moderate size.

Solutions to one-step finite difference analogs of (2.7) are also of the form (2.8), but often exhibit amplification ($|G|>1$) and a different frequency of oscillation (arg $(G) \neq p$). For later discussion we define the amplification factor as $|G|$ and the frequency error factor as the leading terms in the expansion of arg $(G)/p$ in terms of p. $|G|^2$ reflects amplification of energy E, while the scale parameter S in this linear case is a constant.

3. PROPERTIES OF ONE-STEP COMPUTATIONAL METHODS

Table 1 lists and defines the computational methods tested. The names of established methods are stated where known to the author. Nameless methods originated from heuristic considerations and are identified by capital letters. As seen from the table, the first 10 methods required information at only one time step and most were of second-order accuracy. Precise estimates of the truncation error, not shown, were usually smaller when the number of evaluations of $f_i(\chi_1, \ldots, \chi_M; t)$ per time step was increased.

The defining formulas for the methods are indicated in abbreviated form, with $f_i^{(n)}$ standing for $f_i(\chi_1^{(n)}, \ldots, \chi_M^{(n)}; t_0+n\Delta t)$. Euler's modified method was the only implicit method examined. In practice, a variable number of iterations (4–7) were required to produce convergence of this solution. With one iteration, it reduced to the Heun method, which is the "double-forward" approximation used by Lorenz [13]. The Heun method may also be classified as one of the Runge-Kutta family (Hildebrand [7]).

Method A used the "double-forward" estimate of $\chi_i^{(n+1/2)}$ as basis for a subsequent step by a centered difference rule. Method A′ was designed to provide one small time increment $0 \leq \alpha\Delta t \leq \Delta t$ for each fixed double interval $2\Delta t$. In other respects method A′ coincided with method A.

Method B was a simplified version of A in that a single forward difference estimated $\chi_i^{(n+1/2)}$, followed by a centered difference extrapolation. Method C calculated the quadratic terms in f_i following a "geometric-mean" approximation involving $\chi_i^{(n)}$ and a forward difference estimate of $\chi_i^{(n+1)}$; it differed from the Heun method which used an arithmetic average of these quantities.

The Kutta method used forward differences, centered differences, and arithmetic averaging to produce a high order of accuracy.

TABLE 1.—*Defining characteristics of some computational methods for first-order equations. "Steps" denotes the number of initial information time levels required by the procedure. "Order of accuracy" is obtained from a Taylor series analysis.*

Method (description)	Steps	Order of accuracy	Number of f_i evaluations per time step	Formulas or description	Explicit or implicit
One-Step Methods					
1. Euler's modified (trapezoidal)	1	2	≥2	$\chi^{(n+1)}=\chi^{(n)}+\frac{1}{2}[f^{(n)}+f^{(n+1)}]\Delta t$	I
2. Heun (double forward)	1	2	2	$\chi^{(n+1)*}=\chi^{(n)}+f^{(n)}\Delta t$ $\hat{\chi}^{(n+1)}=\chi^{(n)}+\frac{1}{2}[f^{(n)}+f^{(n+1)*}]\Delta t$	E
3. Method A (double forward, centered)	1	2	3	$\chi^{(n+1/2)*}=\chi^{(n)}+f^{(n)}\Delta t/2$ $\hat{\chi}^{(n+1/2)}=\chi^{(n)}+\frac{1}{2}[f^{(n)}+f^{(n+1/2)*}]\Delta t/2$ $\tilde{\chi}^{(n+1)}=\chi^{(n)}+\hat{f}^{(n+1/2)}\Delta t$	E
4. Method A′ (method A; variable Δt)	1	2	3	For even n, $0\leq\alpha\leq 1$, and $\hat{\chi}$ obtained by method 2: $\tilde{\chi}^{(n+\alpha)}=\chi^{(n)}+\hat{f}^{(n+1/2\alpha)}\alpha\Delta t$ $\chi^{(n+2)}=\tilde{\chi}^{(n+\alpha)}+\hat{f}^{(n+1+1/2\alpha)}(2-\alpha)\Delta t$	E
5. Method B (forward, centered)	1	2	2	$\chi^{(n+1/2)*}=\chi^{(n)}+f^{(n)}\Delta t/2$ $\chi^{(n+1)}=\chi^{(n)}+f^{(n+1/2)*}\Delta t$	E
6. Method C	1	2	2	with quadratic $f_i=\sum_{j,k} C_{ijk}\chi_j\chi_k$: $\chi_i^{(n+1)}=\chi_i^{(n)}+\frac{1}{2}\sum_{j,k} C_{ijk}[\chi_j^{(n)}\chi_k^{(n+1)*}+\chi_j^{(n+1)*}\chi_k^{(n)}]\Delta t$, where $\chi^{(n+1)*}=\chi^{(n)}+f^{(n)}\Delta t$.	E
7. Kutta	1	4	4	$\chi^{(n+1/2)*}=\chi^{(n)}+f^{(n)}\Delta t/2$ $\bar{\chi}^{(n+1/2)}=\chi^{(n)}+\bar{f}^{(n+1/2)*}\Delta t/2$ $\chi^{(n+1)**}=\chi^{(n)}+\bar{f}^{(n+1/2)}\Delta t$ $\chi^{(n+1)}=\chi^{(n)}+\frac{1}{6}[f^{(n)}+2f^{(n+1/2)*}+2\bar{f}^{(n+1/2)}+f^{(n+1)**}]\Delta t$	E
8. Method D (two forwards, latest values, reversed variable order)	1	1	2	i assumes successive values $i=1, 2, 3, \ldots, M$: $\chi_i^{(n+1/2)*}=\chi_i^{(n)}+f_i(\chi_1^{(n+1/2)*}, \ldots, \chi_{i-1}^{(n+1/2)*}, \chi_i^{(n)}, \ldots, \chi_M^{(n)})\Delta t/2$, and then with $i'=(M+1-i)$: $\chi_{i'}^{(n+1)}=\chi_{i'}^{(n+1/2)*}+f_{i'}(\chi_M^{(n+1)}, \ldots, \chi_{i'-1}^{(n+1)}, \chi_{i'}^{(n+1/2)*}, \ldots, \chi_1^{(n+1/2)*})\Delta t/2$	E
9. Method D′	1	1	2	Same as D except that order of variables assigned to χ_i is changed randomly before each new time step.	E
10. Euler (forward)	1	1	1	$\chi^{(n+1)}=\chi^{(n)}+f^{(n)}\Delta t$	E
Two-Step Methods					
11. Adams-Bashforth	2	2	1	$\chi^{(n+1)}=\chi^{(n)}+[\frac{3}{2}f^{(n)}-\frac{1}{2}f^{(n-1)}]\Delta t$	E
12. Centered (uncorrected)	2	2	1	$\chi^{(n+1)}=\chi^{(n-1)}+2f^{(n)}\Delta t$	E
13. Centered (correction A)	2	2	1	$\chi^{(n+1)}=\chi^{(n-1)}+2f^{(n)}\Delta t$, periodically corrected by method A of Appendix A	E

Scheme D consisted of two successive operations at each time step, each similar to a forward difference with time increment $\Delta t/2$. Unlike the simple forward difference, the latest estimates of the variables χ_i were used in evaluating f_i.[4] Thus, in the first operation, f_1 would depend only upon the variables $\chi_1^{(n)}, \ldots, \chi_M^{(n)}$; with $\chi_1^{(n+1/2)*}$ determined, f_2 would involve $\chi_1^{(n+1/2)*}, \chi_2^{(n)}, \ldots, \chi_M^{(n)}$. Finally, $\chi_1^{(n+1/2)*}, \ldots, \chi_{M-1}^{(n+1/2)*}, \chi_M^{(n)}$ would determine f_M and hence $\chi_M^{(n+1/2)*}$. The second and final operation consisted of reversing the order in which the variables were solved and then repeating the first operation, starting with the set $\chi_1^{(n+1/2)*}, \ldots, \chi_M^{(n+1/2)*}$ and obtaining $\chi_1^{(n+1)}, \ldots, \chi_M^{(n+1)}$.

From this description it appears that solutions obtained by method D would usually depend upon the order in which the variables were solved. This could be a disadvantage in a grid point or wave number space calculation, for the geometry of the scanning pattern would determine the variable order and hence geometrically bias the solution.

In an attempt to minimize this order bias scheme D′ was invented. It coincided with scheme D except that the order of variables was determined randomly before each new time step. This method appeared to be mainly of academic interest since the programming difficulties would be severe in a system with many degrees of freedom.

The remaining methods shown in table 1 are well known and are useful in later comparisons. The two-step schemes are discussed in section 5 and Appendix A.

[4] This aspect of method D was related to the Gauss-Seidel iterative method of solving linear systems of algebraic equations.

Let us now examine properties of the one-step schemes as shown in table 2. Considering the linear oscillation first, we note that amplification factors for many one-step methods involved p to a power at least equal to 4; higher powers corresponded to increased sensitivity of energy errors to a change in Δt. On the other hand, the frequency error was not so sensitive to Δt, except in the highly accurate Kutta scheme.

Most numerical solutions for the nonlinear case were obtained with 24 time increments per period of oscillation. Comparative energy amplification values were found to be in qualitative accord with those of the linear oscillation. However, the shorter internal time scale of the nonlinear solution produced large quantitative differences. Fractional errors in the scale parameter S were much smaller than those in E, but tended to resemble the E errors. Frequency errors exceeded E errors as in the linear case. However, as expected from earlier remarks, comparative frequency errors were not correctly indicated by the linear results; in some cases the fractional frequency error changed significantly with time.

In view of the linear solution properties it is not surprising that the schemes numbered 2, 5, 6, and 10 were inferior to the other more complicated one-step methods when applied to the nonlinear system. Despite its two part simplicity, scheme D was surprisingly successful in the nonlinear test; as expected, the errors varied with the order in which the three variables were solved. Interestingly, scheme D′ with randomized order was comparatively poor.

Results for method A′ showed that, given an average value of Δt, the use of variable time increments resulted in

TABLE 2.—*Properties of one-step computational methods taken from linear analysis and the numerical solutions of nonlinear equations. All numerical values are estimates based upon the first several cycles. Numerical values estimated from linear oscillations with the same period as the nonlinear oscillation are shown in parentheses.*

Method	Linear periodic solution		Nonlinear periodic solution							
	Amplification factor $\lvert G\rvert$	Frequency error factor	$\frac{\Delta t}{\text{period}}$	$10^3\times$net fractional energy error per cycle		$10^3\times$net fractional frequency error per cycle		$10^4\times$net fractional scale error per cycle	
1. Euler's modified	1	$(1-p^2/12+\ldots)$	1/24	$\leq+.028$	(0)	+46.	(−5.7)	$\leq+.18$	(0)
2. Heun	$(1+p^4/4)^{1/2}$	$(1+p^2/6+\ldots)$	1/24	+164.	(+28.)	+162.	(+11.)	+4.9	(0)
			1/48	+13.	(+3.4)	+104.	(+3.)	+0.6	(0)
3. Method A	$(1+p^6/64)^{1/2}$	$(1+p^2/24+\ldots)$	1/24	+0.48	(+0.12)	+64.	(+2.8)	+0.23	(0)
4. Method A′:									
General α	$(1+\alpha^6p^6/64)^{1/4}\times(1+(2-\alpha)^6p^6/64)^{1/4}$	$(1+p^2(1/6-\alpha/4+\alpha^2/8)+\ldots)$							
$\alpha=1.0$	$(1+.0156p^6)^{1/2}$	$(1+.0417p^2+\ldots)$	1/24	+0.48	(+0.12)	+64.	(+2.8)	+0.23	(0)
$\alpha=0.8$	$(1+.0254p^6+\ldots)^{1/2}$	$(1+.0467p^2+\ldots)$	1/24	+0.75	(+0.19)	+62.	(+3.2)	+0.35	(0)
$\alpha=0.6$	$(1+.0592p^6+\ldots)^{1/2}$	$(1+.0617p^2+\ldots)$	1/24	+1.6	(+.45)	+53.	(+4.2)	+0.86	(0)
$\alpha=0.0$	$(1+.5000p^6+\ldots)^{1/2}$	$(1+.1667p^2+\ldots)$	1/24	+16.	(+3.8)	variable: +70. to −180.	(+11.4)	+7.	(0)
$0\leq\alpha\leq1$ picked randomly	$(1+.1429p^6+\ldots)^{1/2}$	$(1+.0834p^2+\ldots)$	1/24	+14.	(+1.1)	variable: +90. to −180.	(+5.7)	+2.3	(0)
5. Method B	$(1+p^4/4)^{1/2}$	$(1+p^2/6+\ldots)$	1/24	+158.	(+28.)	+167.	(+11.)	+5.5	(0)
6. Method C	$(1+p^4/4)^{1/2}$	$(1+p^2/6+\ldots)$	1/24	+110.	(+28.)	+125.	(+11.)	+5.7	(0)
7. Kutta	$(1-p^6/72)^{1/2}$	$(1+p^4/8+\ldots)$	1/24	−0.81	(−0.12)	+58.	(+.59)	−0.20	(0)
8. Method D:									
order of solution of variables:									
$(\theta_W, \theta_Z, \psi_W)$	1	$(1+p^2/24+\ldots)$	1/24	+.000	(0)	+54.	(+2.8)	+.000	(0)
$(\psi_W, \theta_W, \theta_Z)$	1	$(1+p^2/24+\ldots)$	1/24	+.000	(0)	+67.	(+2.8)	+.000	(0)
$(\theta_Z, \psi_W, \theta_W)$	1	$(1+p^2/24+\ldots)$	1/24	+.000	(0)	+67.	(+2.8)	+.000	(0)
9. Method D′:									
random variable order	1	$(1+p^2/24+\ldots)$	1/24	+6.7	(0)	+410.	(+2.8)	variably large: ≈50.	(0)
10. Euler	$(1+p^2)^{1/2}$	$(1-p^2/3)$							
severe instability commenced at:									
cycle 0.7			1/24	+2,040.	(+3,642.)	+80.	(−22.8)	+300.	(0)
cycle 1.7			1/48	+1,880.	(+1,200.)	+46.	(−5.7)	+100.	(0)
cycle 2.7			1/72	+875.	(+690.)	+60.	(−2.5)	+90.	(0)
cycle 4.0			1/96	+562.	(+480.)	+58.	(−1.4)	+72.	(0)

increased computational errors for both linear and nonlinear oscillations when applied to method A. Linear analysis suggests that this conclusion is valid for other one step schemes as well.

Thus, the outstanding one-step methods were those numbered 1, 3, 7, and 8. Further information on these was given by the maximum local errors in E and S. These errors, not shown in table 2, were confined to the quick transition periods of the nonlinear solution. They were much larger than the net error in the case of Euler's modified method, despite the increased number of iterations per time step during the transition. On the other hand, the Kutta method exhibited excellent stability in this sense, as expected from its small local truncation error.

4. TIME RESOLUTION VS. COMPLEXITY OF ONE-STEP METHODS

We have noted that those one step schemes which were most simply calculated at each time step were predictably poor compared to more complicated schemes. However, a natural question is whether a simple one-step scheme used with smaller time increments can compete favorably with these more sophisticated ones.

To test this, four experiments using the simple Euler (forward difference) method with successively smaller values were performed. With 48 time increments per period, the Euler scheme required about as much computational time as each of the schemes 2, 5, 6, 8, or 9 required with only 24 increments per period. From table 2 we see that the performance of each of the latter methods was clearly superior to the Euler method in this case. Similar "equal computational time" comparisons made with three part schemes 3, 4, and 7 lead to the same conclusion. Thus, the Euler method appears inferior to more complex one step schemes even when it is used with smaller time increments.

An additional experiment was next performed with the Heun method rather than the Euler method. The time resolution was increased to 48 increments per oscillation and results were compared with those of method A used with 24 increments per period. It is seen in table 2 that method A was superior to the simpler Heun method while demanding only ¾ as much computational time.

Based on these results it appears that increased time resolution is not the most efficient way to decrease computational errors for one-step schemes. Instead, as suggested by the amplification factors for linear oscillations, accuracy is usually achieved by increasing the number of f_i evaluations per time step.

5. TWO-STEP METHODS

The results discussed in sections 3 and 4 were confined to one-step methods. To put these in better perspective we now examine the results of similar tests on the commonly used two-step methods defined in table 1.

We first note that the "extra" time level $(n-1)$ appeared solely in the function $f_i^{(n-1)}$ for the Adams-Bashforth scheme; only $f_i^{(n)}$ was evaluated in the centered method. This difference was reflected in the solutions to the linear system. For the centered method the solution was

$$\chi^{(n)}=\eta_1 e^{i\theta n}+\eta_2(-1)^n e^{-i\theta n} \tag{5.1}$$

where $\tan\theta=p(1-p^2)^{-1/2}$. η_1 and η_2 were constants which could be determined by $\chi^{(n)}$ and $\chi^{(n-1)}$; Lilly [10] gave their approximate form for a special case.

The first term in (5.1) corresponds to the "physical mode" of the solution, modified by computational errors. The second term is the extraneous "computational mode"

TABLE 3.—*Properties of two-step computational methods taken from linear analysis and the numerical solutions of nonlinear equations. All numerical values are estimates based upon the first several cycles. Numerical values estimated from linear oscillations with the same period as th nonlinear oscillation are shown in parentheses. Values for the nonlinear oscillation are classified according to estimated "physical mode" and "computational mode" contributions.*

Method	Linear Periodic Solution		Nonlinear Periodic Solution						
				Physical mode			Computational mode		
	Amplification factor $\|G\|$	Frequency error factor	$\frac{\Delta t}{\text{period}}$	$10^3\times$net fractional energy error per cycle	$10^3\times$net fractional frequency error per cycle	$10^4\times$net fractional scale error per cycle	$10^3\times$max. fractional energy error per cycle	$10^4\times$max. fractional scale error per cycle
11. Adams-Bashforth	$(1+p^4/4+\ldots)^{1/2}$	$(1+5/12\,p^2+\ldots)$						
(severe instability at cycle 1.6)			1/24	+445. (+28.)	+158. (+27.6)	+34. (0)	0.	0.
			1/48	+25.5 (+3.4)	+101. (+6.9)	+0.84 (0)	0.	0.
			1/72	+6.45 (+1.0)	+57. (+3.1)	+0.43 (0)	0.	0.
12. Centered	1	$(1+p^2/6)$						
(uncorrected)								
(instability beyond cycle 20)			1/24	bounded by +120. (0)	+82. (+11.)	bounded by +65. (0)	398.	810.
			1/48	bounded by +24. (0)	+70.2 (+3.)	bounded by +7.5 (0)	190.	410.
			1/72	bounded by +12. (0)	+62.5 (+1.2)	bounded by +2.5 (0)	110.	230.
13. Centered	1	$(1+p^2/6)$						
(correction A applied each 24 steps)								
(severe instability at cycle 5.7)			1/24	bounded by +136. (0)	+167. (+11.)	bounded by −50. (0)	330.	360.
			1/48	bounded by +6.8 (0)	+69. (+3.)	bounded by −1.36 (0)	53.	110.
			1/72	bounded by +12.0 (0)	+63. (+1.2)	bounded by +.80 (0)	2.5	77.

introduced by the increased order of the finite difference method. A characteristic of this mode is its sign alternation at successive time steps. For the centered method, (5.1) shows that the maximum size of the computational mode never decreases as n increases. This is not the case for the Adams-Bashforth method, where the maximum amplitude can be shown to decrease as p^n. Thus, problems of "starting" and correcting the solution in order to reduce the amplitude of the computational modes appear important only in the case of centered differences. These topics are discussed in Appendix A.

Table 3 presents the quantitative results obtained for the two-step methods. All solutions were started with the values $\chi^{(0)}$ and $\chi^{(1)}$ taken from the exact solution (equation (2.3)); as discussed in Appendix A, this procedure does not completely exclude the computational mode initially.

We first note that computational mode oscillations (of period $(2\Delta t)$) never appeared in the nonlinear case using the Adams-Bashforth method. On the other hand, such fluctuations in E and S were apparent with the centered methods, and usually exceeded those associated with the physical mode. Correction of the centered method by procedure A did reduce the computational mode, but to a lesser extent than that expected from the linear solutions.

The remainder of table 3 concerns the characteristics of the physical mode; its errors are the counterparts of those discussed for the one-step schemes in sections 3 and 4. We first note that the frequency errors exceeded the amplitude errors for linear oscillations as in the one-step methods. This was also true for the nonlinear solutions when the time increments were small; with larger increments the reverse was true, and in two instances severe computational instability resulted.

Comparison with table 2 shows clearly that, for a given Δt, these two-step methods usually produced larger errors in the physical mode than the one-step schemes. However, considered on an "equal computational time" basis (as in section 4) the standings of the two-step methods improved. For example, their performance generally surpassed that of the poorer one-step methods 2, 5, 6, or 10. Nevertheless, the two-step methods remained generally inferior to the outstanding one-step methods 3 and 8 in this case.

Table 3 also allows intracomparison of physical mode errors for the two-step methods. In the cases of largest Δt values, the Adams-Bashforth and "corrected-centered" methods were rather poor. However, with smaller Δt values they represented a slight improvement over the "uncorrected-centered" method. Considering also the large computational mode errors of the centered schemes, one must conclude that the Adams-Bashforth and "corrected-centered" schemes were superior to the "uncorrected-centered" method.

6. CONCLUDING REMARKS

We have examined the properties of computational schemes applied to a spectral baroclinic model of maximum simplicity whose linear and nonlinear characteristics were known. The performance of computational methods for the linear oscillation was found to be a better indicator of the nonlinear properties than the order of truncation error. However, the truncation error was useful in assessing local errors associated with sudden nonlinear changes in the solution. Largest fractional errors were usually found in the frequency, followed by successively smaller ones in the amplitude and spatial spectrum.

For the one-step methods, reduction of long-term errors was usually accomplished most effectively by increasing the number of calculations of the time derivatives at each time step rather than reducing the time increment Δt. The best one-step methods were found to be a four part Kutta scheme, the three-part scheme A, Euler's modified implicit scheme, and a two-part scheme which utilized the latest values of each ordered variable. Other two-part methods produced larger errors. Also, the use of variable time increments with method A usually resulted in increased local and propagated errors for both types of oscillations.

The two-step methods produced physical mode errors which were generally larger than most one-step methods with the same time increment. In fact, these two step schemes compared favorably only when their computational time advantage was sacrificed by using a reduced time increment. In this case, the best of these two-step methods (Adams-Bashforth) was still somewhat inferior to the best one-step methods when compared on an "equal computation time" basis. In all cases both the corrected and uncorrected versions of the centered difference scheme developed relatively large "computational mode" oscillations during the nonlinear phases of the oscillation.

The above conclusions should be accepted with a note of caution. They have been conveniently obtained through study of a small component model. Thus, their validity for systems with many more degrees of freedom is not assured. For example, a large geophysical system undergoing irregular oscillations possesses a variety of individual frequencies which are sustained by nonlinear energy exchanges involving triads of elements similar to that found in section 2. The mechanisms of these transfers are frequency dependent (Phillips [16]), so an accurate portrayal of the fluctuations would demand a numerical scheme with small frequency errors as well as small amplitude errors. Most schemes do not satisfy both of these requirements. This suggests that detailed climatic or energetic studies may require multipart, one-step schemes, probably from the Runge-Kutta family.

APPENDIX A.—STARTING AND CORRECTION PROCEDURES FOR CENTERED DIFFERENCES

The purpose of this appendix is to discuss some procedures for reducing the amplitude of the computational mode associated with the centered difference scheme.

It is convenient to begin with the linear theory. As mentioned in section 5, η_1 and η_2 are determined by $\chi^{(n)}$,

$\chi^{(n-1)}$ and equation (5.1). At the beginning of the computation these relations are given by:

$$\eta_1=(\chi^{(0)}e^{-i\theta}+\chi^{(1)})/(2\cos\theta)$$

$$\eta_2=(\chi^{(0)}e^{+i\theta}-\chi^{(1)})/(2\cos\theta). \tag{A.1}$$

Since the initial conditions $\chi^{(0)}$ are known exactly, $\chi^{(1)}$ alone determines η_1 and η_2. The method by which $\chi^{(1)}$ is estimated from $\chi^{(0)}$ may be termed the "starting method."

The tests discussed in section 5 were all started using the "exact" value of $\chi^{(1)}$; in this way, it was believed that initial errors would be minimized. However, this procedure does not eliminate the computational mode completely. This may be seen in the linear case, where the exact solution gives

$$\chi^{(1)}=\chi^{(0)}e^{ip}. \tag{A.2}$$

Substitution into (A.1) shows that $\eta_2=\chi^{(0)}(ip^3/12+\cdots)$, and is not zero. This is a characteristic of other multistep schemes ([7], p. 207), and apparently arises because the phase error $(\theta-p)$ of the centered scheme is not zero. Equations (A.2) and (A.1) also yield $\eta_1=\chi^{(0)}[1-ip^3/12+\cdots]$; the associated amplitude error is $O(p^6)$ while the phase error is $O(p^3)$.

These results may be compared with those of the more common starting method which uses a forward difference to estimate $\chi^{(1)}$:

$$\chi^{(1)}=\chi^{(0)}(1+ip). \tag{A.3}$$

From (A.1) we then obtain

$$\eta_2=-\chi^{(0)}\left(\frac{p^2}{4}+\cdots\right),\ \eta_1=\chi^{(0)}\left(1+\frac{p^2}{4}+\cdots\right).$$

Thus, use of the forward difference in place of the "exact" value produces an initial computational mode amplitude larger by a factor of $(3/p)$. It also produces a larger amplitude error in the physical mode, of $O(p^2)$.

Unfortunately, amplification of the computational mode frequently develops spontaneously in the nonlinear solutions, so that starting procedures alone seem inadequate. In such cases correction procedures may be periodically applied to reduce the computational mode. Two such methods will now be discussed.

"Correction A" was used in the tests discussed in section 5. It consisted of first averaging the centered difference solutions $\chi^{(n)}$ and $\chi^{(n-1)}$, followed by forward and backward differences to give the "corrected" values $\hat{\chi}^{(n)}$ and $\hat{\chi}^{(n-1)}$:

$$\overline{\chi}^{(n-1/2)}=\tfrac{1}{2}[\chi^{(n)}+\chi^{(n-1)}]$$

$$\hat{\chi}^{(n)}=\overline{\chi}^{(n-1/2)}+\overline{f}^{(n-1/2)}\Delta t/2$$

$$\hat{\chi}^{(n-1)}=\overline{\chi}^{(n-1/2)}-\overline{f}^{(n-1/2)}\Delta t/2. \tag{A.4}$$

When (A.4) was applied to the linear system, the "corrected" values $\hat{\eta}_1$ and $\hat{\eta}_2$ were found in terms of the original quantities η_1 and η_2. In this case the results could be expressed as

$$\frac{|\hat{\eta}_2|}{|\eta_2|}<\frac{|\eta_1|}{|\eta_2|}\,[O(p^3)]+[O(p^4)] \tag{A.5}$$

and

$$\frac{|\hat{\eta}_1|}{|\eta_1|}<[1+O(p^2)]+\frac{|\eta_2|}{|\eta_1|}\,[O(p)]. \tag{A.6}$$

Inequality (A.5) indicates that the correction would reduce the computational mode amplitude when it was originally large enough ($|\eta_2|>|\eta_1|O(p^3)$). However, this correction could increase the computational mode when it was initially small enough ($|\eta_2|<|\eta_1|O(p^3)$). Inequality (A.6) indicates that the correction procedure would usually introduce a small ($O(p^2)$) error into the physical mode.

Let us now consider "correction B," which was not used in section 5. It consisted of using backward and forward differences from the respective centered difference solutions $\chi^{(n)}$ and $\chi^{(n-1)}$, followed by averaging of the two estimates then available at each time level:

$$\chi^{(n-1)*}=\chi^{(n)}-f^{(n)}\Delta t$$

$$\chi^{(n)*}=\chi^{(n-1)}+f^{(n-1)}\Delta t$$

$$\hat{\chi}^{(n-1)}=\tfrac{1}{2}[\chi^{(n-1)}+\chi^{(n-1)*}]$$

$$\hat{\chi}^{(n)}=\tfrac{1}{2}[\chi^{(n)}+\chi^{(n)*}]. \tag{A.7}$$

Application of this procedure to the linear system (2.6) gave results nearly the same as those expressed in (A.5, A.6) for correction A.

Finally, corrections A and B were applied to the nonlinear system for the case with 24 time increments per cycle; the results may be seen in table A1. We first note that both procedures appear to have encouraged a severe computational instability in the physical mode while suppressing the computational mode. However, this distressing behavior was not true of correction A in cases with smaller time increments (see section 5).

On the basis of table A1, correction A appears slightly superior to the correction B in its ability to follow the physical mode. With respect to computational mode oscillations in E and S, correction A was a nearly perfect damping agent. Correction B damped only about 95 percent of these energy oscillations. For this reason correction A was chosen for the tests of section 5.

TABLE A1.—*Time of commencement of severe computational instability for centered differences corrected by methods A and B. Time is given in cycles. $\Delta t=1/24$ period in all cases.*

Number of steps between corrections	Method A	Method B
12	2.8	3.1
24	5.7	3.5
48	10.0	6.1
96	5.3	5.0
192		8.3
No correction	>20.0	>20.0

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